A toy model for multi-dimensional cellular detonations

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1 Introduction

The first attempt at a reduced qualitative description of detonations is due to Fickett [4, 5], who introduced a toy model as a vehicle to better understanding the intricacies of detonation theory. Several other researchers have similarly taken a qualitative approach. Majda, for example, focused on the effect of viscosity on the combustion waves, and showed through a simplified model that a theory analogous to the ZND theory exists for viscous detonations [9] in his toy model. Radulescu and Tang [11] have recently demonstrated that a simple extension of Fickett's model can capture not only ZND-like solutions, but also much of the unsteady dynamics of one-dimensional detonations. In [3, 7], we have shown that a model as simple as a scalar forced Burgers equation contains all the ingredients necessary to reproduce the dynamical richness of one-dimensional detonations, including a complex linear stability spectrum and chaos.

All these prior works, however, are limited to one-dimensional phenomena. Because gaseous detonations are generally multi-dimensional, it is of interest to obtain a model that can qualitatively reproduce observed cellular structures. Here, we propose and analyze such a two-dimensional model. It extends the scalar one-dimensional model consisting of the forced Burgers equation that we introduced in [7]. We show that the extended model captures some of the multi-dimensional nature of detonations waves. The linear stability problem for the model is analyzed by means of the Laplace transform. It is observed that the maximum growth rate typically occurs at a nonzero transverse wave number, which therefore dominates the early growth of instability. By means of numerical simulations, we also show that solutions of the toy model tend, in the long-time limit, to form multi-dimensional patterns reminiscent of detonation cells.

2 The two-dimensional analog

As a starting point, we take the one-dimensional model introduced in [7],

$$u_t + \frac{1}{2}\left(u^2\right)_x = f\left(x - x_s, u_s\right), \tag{1}$$

where u is a velocity-like variable, x_s denotes the x position of the detonation shock and u_s denotes the state of u immediately after the shock. Subscripts t and x here (and ξ, y below) denote partial differentiation. In order to extend equation (1) to two dimensions we need, as a minimum, another variable, v, analogous to the transverse velocity, and a relation between u and v. Our extension is motivated by the asymptotic form of weakly curved hyperbolic waves, where the dependence on the transverse direction is typically linear, and reinforces the fact that weakly nonlinear quasi-planar waves generate no vorticity to leading order. We thus propose the following two-dimensional model:

$$u_t + \frac{1}{2}\left(u^2\right)_x + v_y = f(x - x_s, u_s), \tag{2}$$
$$v_x - u_y = 0. \tag{3}$$

Because (2-3) is not derived by any rational approximation of a physical system, its full justification comes *a posteriori* by investigating its properties. However, the model is related to a weakly nonlinear multi-dimensional asymptotic theory, which although harder to analyze, can be obtained by a systematic reduction of the reactive Euler equations [2].

For the purpose of the forthcoming calculations, it is convenient to rewrite (2-3) in a shock-attached reference frame. We represent the shock position by the zero-level set of $\psi = x - s(y,t)$, where $s(y,t)$ is assumed to be a single valued function giving the x position of the shock. Then, in terms of $\xi = x - s(y,t)$, (2-3) becomes

$$u_t + (u - s_t)u_\xi + v_y - s_y v_\xi = f(\xi, u_s), \tag{4}$$
$$u_y - s_y u_\xi - v_\xi = 0. \tag{5}$$

The quantities s_t and s_y are related to the state at the shock by the jump conditions given by

$$s_t\left[u\right] - \frac{1}{2}\left[u^2\right] + s_y\left[v\right] = 0, \tag{6}$$
$$s_y\left[u\right] + \left[v\right] = 0, \tag{7}$$

where $[\cdot]$ represents the jump of an enclosed quantity across the shock. Equations (2-3), together with the jump conditions (6-7), constitute our main model.

3 Traveling wave solutions and stability analysis

For the two-dimensional system, we are interested in the stability properties of ZND waves with respect to transverse perturbations, and in the full nonlinear dynamics of the system. Assuming that the state ahead of the shock is given by $u = 0,\ v = 0$, we obtain the one-dimensional solution from (2-3) as

$$u_0(\xi) = \frac{u_{0s}}{2} + \sqrt{\frac{u_{0s}^2}{4} - 2\int_x^0 f\left(z, u_{0s}\right) dz}, \qquad v_0(\xi) = 0, \tag{8}$$

where $u_{0s} = 2D$ represents, by the jump conditions, the steady-state shock velocity. We require $u_{0s} = \zeta\left(2\sqrt{2\int_{-\infty}^0 f\left(y, u_{0s}\right) dy}\right)$, with the overdrive factor $\zeta \geq 1$. If $\zeta = 1$ (CJ case), then the characteristics at the end of the reaction zone (when $f = 0$) are sonic relative to the lead shock. When $\zeta > 1$, detonations move faster than the CJ wave. In overdriven detonations, characteristics from $-\infty$ catch up with the lead shock in finite time and affect its dynamics. The larger the overdrive, the closer a detonation wave looks to an inert piston-induced shock, and therefore in the limit of large overdrive, detonations are expected to be stable.

We consider now the multi-dimensional linear stability of solutions given by equation (8). Linearization leads to

$$u_{1t} + c_0 u_{1\xi} + u_0' u_1 + v_{1y} = b_0 u_{1s}, \tag{9}$$
$$u_{1y} - v_{1\xi} = -u_{0\xi} v_{1s}/u_{0s}, \tag{10}$$

where $c_0,\ b_0,\ u_{0s}$ are functions of the steady-state profile given by $c_0 = u_0 - u_{0s}/2$, $b_0 = \partial f/\partial u_s\,(x, u_{0s}) + u_0'/2$, and $u_{1s} = u_1(\xi = 0^-, y, t)$, $v_{1s} = v_1(\xi = 0^-, y, t)$ denote the perturbed quantities evaluated immediately after the shock. Here subscript 0 indicates the base steady solution and 1 the perturbation. We solve the linearized system by means of the Laplace transform in time following closely [1]. For example, in the one-dimensional case, the dispersion relation is found to be

$$c_0(0) = \int_{-\infty}^{0} b_0(z) \exp\left[-\sigma p(z)\right] dz, \tag{11}$$

which is the same as the one obtained by means of normal modes (here, σ is the Laplace transform variable). Therefore, in the context of the simple toy model presented here, both Laplace transform and normal modes yield the same stability criterion.

4 Multi-dimensional dynamics

In this section, we study the properties of (2-3) for the same choice of f as given in [3]. Upon appropriate rescaling of the variables as in [3], we obtain the dimensionless system

$$u_t + \frac{1}{2}\left(u^2\right)_x + v_y \quad = \quad f(x - x_s, u_s), \tag{12}$$
$$v_x - u_y \quad = \quad 0. \tag{13}$$

where f is defined as,

$$f(x - x_s, u_s) = \frac{1}{4\zeta^2\left(1 + \text{Erf}\left[\frac{u(0,t)^{-\alpha}}{2\sqrt{\beta}}\right]\right)} \frac{1}{\sqrt{4\pi\beta}} \exp\left[-\frac{\left(x - x_s + \left(u\left(0,t\right)\right)^{-\alpha}\right)^2}{4\beta}\right]. \tag{14}$$

The same three parameters, α, β, and ζ, as found in [7] are again seen in f. They represent, respectively, the sensitivity of the reaction rate to variations at the shock, the ratio of the lengths of the reaction zone to the induction zone, and the degree of overdrive. The overdrive ζ is seen to simply scale the amplitude of the source term, with the effect of the forcing going to zero as $\zeta \to \infty$. We show in figure 1 the effect of the overdrive factor on the steady detonation profile. For large enough overdrive, the wave is almost constant, being sustained primarily by the imposed left boundary condition. The linear stability spectrum of (12-13) is obtained by means of Laplace transform. As can be shown, the poles of the Laplace transform (corresponding to instabilities should they lie on the right half of the complex plane) are given by the zeros of the stability function

$$R(\sigma, \ell) = \boldsymbol{\theta}_1(0) \cdot \begin{bmatrix} \sigma \\ \frac{i\ell}{2} \end{bmatrix} - \int_{-\infty}^{0} \boldsymbol{\theta}_1 \cdot \begin{bmatrix} \sigma b_0/c_0 \\ \frac{i\ell u_{0s}}{2} u_0' \end{bmatrix} dz. \tag{15}$$

Here $\boldsymbol{\theta}_1$ is the bounded solution of the appropriate adjoint homogeneous problem, and l is the transverse wavenumber. The main difficulty with numerically solving for the roots of R is that, in general, $\boldsymbol{\theta}_1$ cannot be found analytically. Therefore, each single evaluation of $R(\sigma, \ell)$ requires solving a system of linear

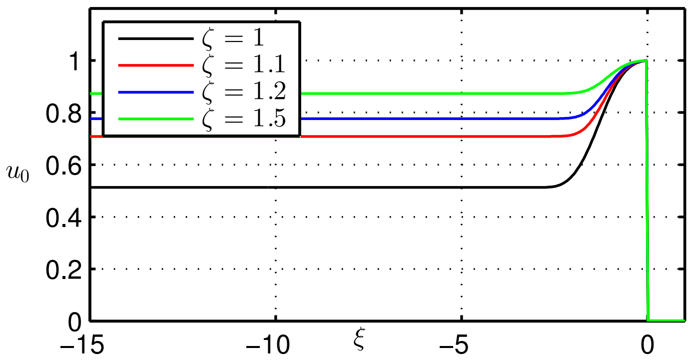

Figure 1: Steady-state solution profiles for (2-3) as the overdrive is varied while keeping all other parameters fixed.

ODEs with variable coefficients to obtain $\boldsymbol{\theta}_1$ and evaluating the integral $\int_{-\infty}^{0} \boldsymbol{\theta}_1 \cdot \begin{bmatrix} \sigma b_0/c_0 \\ \frac{i\ell u_{0s}}{2} u_0' \end{bmatrix} dz$. This can be quite costly, especially when performing a parametric study for varying α and β. We investigate first the effect of the overdrive on the stability of the wave. As discussed before, based on the simple physical argument that overdriven detonations are closer to inert shocks, we expect the overdrive to have a stabilizing effect. This is confirmed in figure 2(a), where we plot the growth rate, σ_r, as a function of the transverse wave number, ℓ, for $\beta = 0.1,\ \alpha = 4.05$, and increasing overdrive $\zeta = 1.05, 1.1, 1.2$. We see that the overdrive factor indeed has a stabilizing effect. We also observe that certain transverse waves are more unstable than purely longitudinal disturbances ($\ell = 0$), and therefore we expect multi-dimensional effects to play a role even when the traveling wave is stable to one-dimensional perturbations.

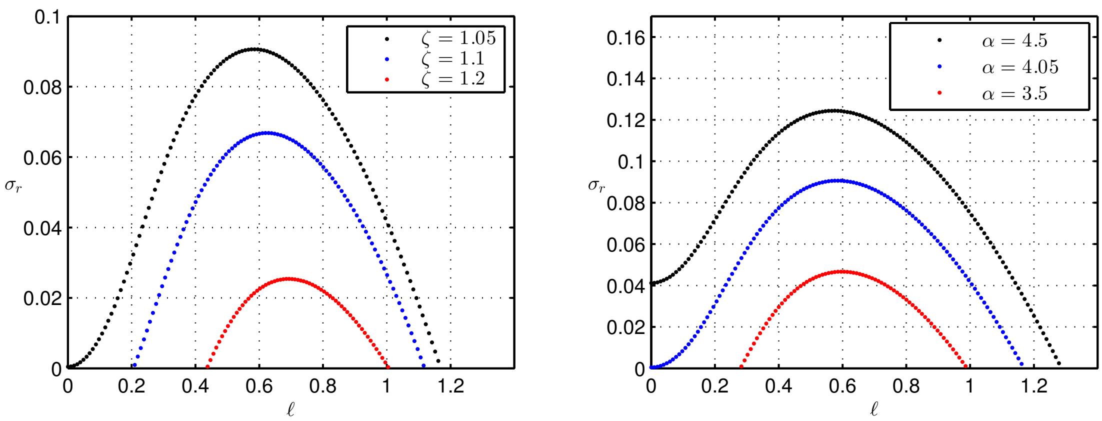

Figure 2: (a) Dispersion relation for $\beta = 0.1$, $\alpha = 4.05$, and varying degree of overdrive. (b) Dispersion relation for $\beta = 0.1$, $f = 1.05$, and varying α.

We also study the effect of α on the stability of the traveling waves. Since α measures the sensitivity of the forcing to changes in the steady traveling wave speed, we expect larger values of α to correspond to more unstable waves. In particular, we expect the growth rate of the perturbations, σ_r, to increase with α. This is precisely what is observed in figure 2(b), where we display the effect of α on the multi-dimensional stability of the wave. We notice that α seems to have very little effect on the most unstable transverse mode, and for the parameters plotted in figure 2(b), the most unstable wavenumber is given by $\ell \approx 0.6$, regardless of the value of α. This is consistent with the one-dimensional picture, where we found that α had very little effect on the imaginary part of the unstable eigenvalues.

These linear stability results suggest that two-dimensional effects play an important role in the ZND waves. Next we investigate, by means of numerical simulations, what happens after the onset of instabilities. The numerical algorithm employed to solve (2-3) is based on a semi-implicit time discretization and is explained in detail in [2]. We show here that the toy model exhibits some of the interesting structures of real multi-dimensional detonations. All numerical simulations are initialized with the ZND solution. The equations are solved in an inertial frame of reference moving with constant speed $D = 1/2$, which is the dimensionless speed of the ZND wave. The top and bottom boundary conditions are that of a wall. We employ an inflow boundary condition on the right and an outflow on the left.

If the ZND wave is only weakly unstable (meaning the parameters are close to the neutral stability boundary), very regular multi-dimensional patterns are observed, which at a qualitative level match rather well with cellular patterns observed in gaseous detonations in dilute mixtures [6, 8, 10]. We see the appearance of certain regions where the induction zone, measured by the distance between the shock and the peak of f, is significantly reduced, and in these regions the energy is released shortly after the lead shock. In contrast to real detonations, however, the transverse waves here appear to be smooth.

With varying degree of overdrive, we notice that waves which are near the Chapman-Jouguet case are more unstable, with stronger transverse variations. It also appears that for smaller overdrive the cells become larger. Both of these findings are consistent with the linear stability predictions, shown in figure 2, where it can be seen that (1) smaller ζ corresponds to larger growth rates, and (2) the wavelength of the most unstable eigenvalue increases with decreasing degree of overdrive.

Finally, in figure 3 we show the result of our experiment with the effect of α on the stability and structure of the detonation wave. We see that, as in the one-dimensional case, larger values of α lead to more complex dynamics. In particular, we observe that by increasing α to a large-enough value, the patterns become more complex, up to the point where no regularity can be easily identified (figure 3(c-d)).

Unlike the one dimensional case studied in [3, 7], quantitatively characterizing two-dimensional dynamics is more challenging. It does seem, however, that the solutions go through some sort of bifurcation, where the transverse waves go from having one maximum (figure 3(a-b)), to two maxima (not shown), to apparently many (figure 3(c-d)). Further quantitative study of this model will be presented elsewhere.

5 Conclusions

We have introduced a two-dimensional extension of the toy model proposed in [3, 7]. The multi-dimensional linear stability properties of the traveling wave solutions were analyzed by means of Laplace transform. It was shown that the dispersion relation consists of an integral equation, much like the explicit formula derived for the one-dimensional detonations in [3]. Evaluation of the dispersion relation is a computationally expensive procedure, where solutions of the homogeneous adjoint problem have to be found for each evaluation of the dispersion relation. It was shown that, akin to detonations in the reactive Euler equations, the overdrive factor has a stabilizing effect on the traveling wave. We also show by numerical simulations that solutions of (2-3) contain multi-dimensional structures of varying complexity. In particular, we observed that very regular cells tend to form when the parameters are near the stability boundary, and that the further we get from the stability boundary, the more irregular the patterns become.

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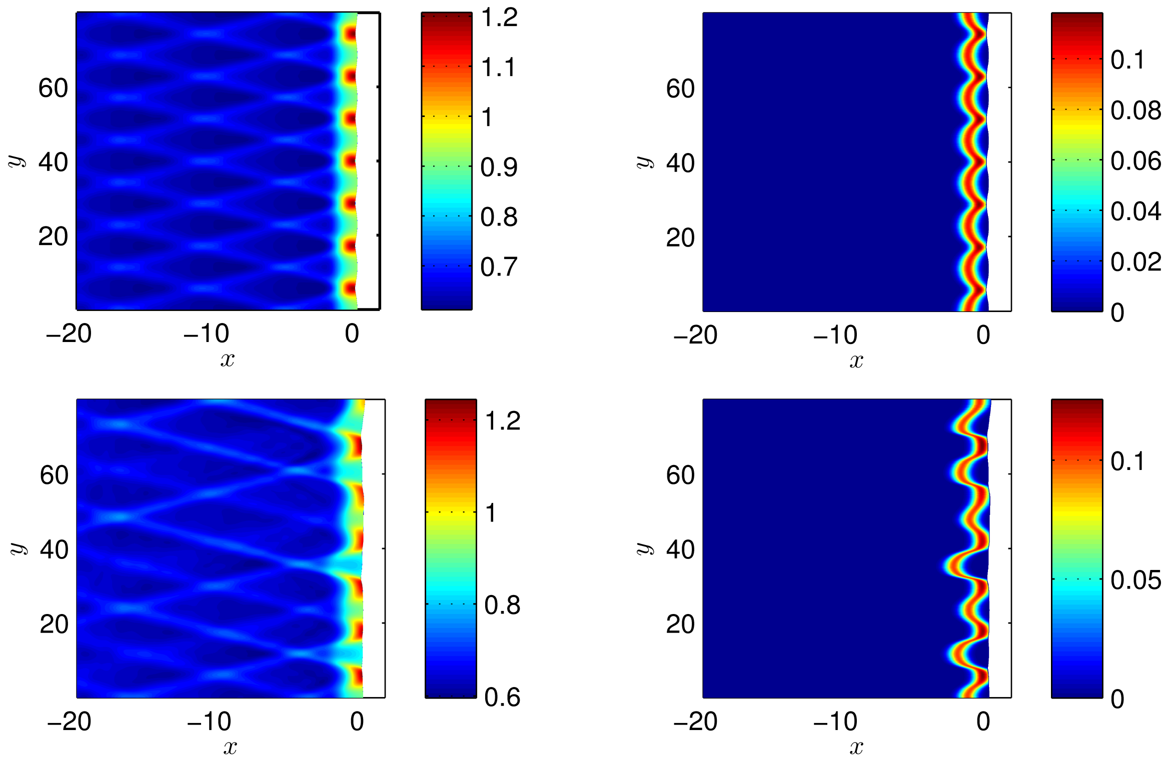

Figure 3: Large time behavior of two-dimensional solutions. The parameters are $\zeta = 1.05$, $\beta = 0.1$, $\alpha = 4.05$ (top), and $\alpha = 4.5$ (bottom). On the left, u is displayed and on the right, f.

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